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THEORETICAL PREDICTION
OF VIBRATIONAL CIRCULAR DICHROISM
OF HEXOSES IN LINEAR FORM

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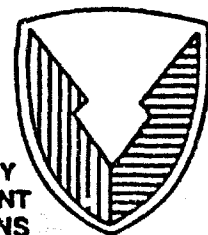Bethlehem, PA 18015-3172

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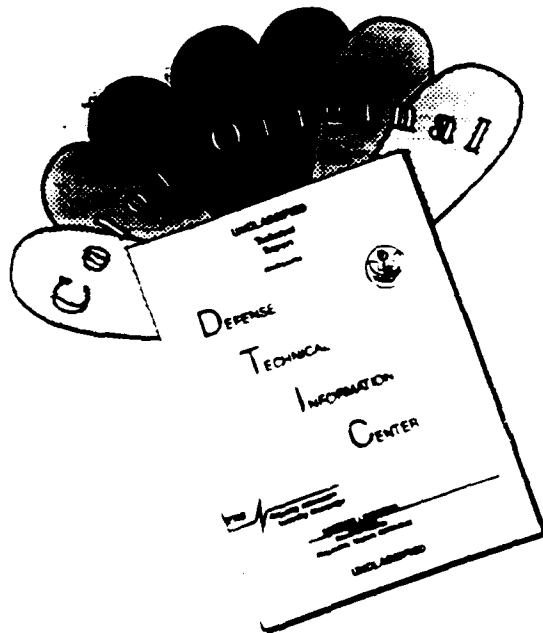June 1992

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We predict vibrational circular dichroism (VCD) of the 6-carbon dextrarotatory compounds: allose, altrose, mannose, glucose, idose, gulose, talose, and galactose with the objective of training a polarization sensitive remote detector to accurately sense these and similar chiral materials in the field. The line of thinking currently being followed for biological detection is that chiral biologicals and sugars react to circularly polarized light in a similar manner. The procedure for computing VCD in the hexoses involves optimization of geometries at the 3-21G level using Gaussian 90 and the subsequent determination of normal mode frequencies and rotational strengths based on the method of P.J. Stephens, which is incorporated in the cambridge analytical derivative package program version 4.2. All calculations were performed on STARDENT 3000 computers. Key results to be reported include optimized structures, frequencies, rotational strengths, and progress toward incorporating scaled force fields into the procedure.

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PREFACE

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1. INTRODUCTION

In this report studies on the theoretical prediction of the VCD spectra of hexoses (sugars with 6 carbon atoms) are summarized. In addition, the current status of scaling of the force field of a molecule and the relation of the scaled force field to VCD parameters for sugars is briefly discussed. This report builds on work presented in two previous reports (1,2). The interested reader is also referred to several key studies on VCD reported in the literature (3-11).

The work that is presented in this report should dovetail with the experimental program on Mueller Matrix Spectroscopy using phase enhanced modulation which is under the direction of one of the coauthors (AHC). The predicted VCD spectra is related to the (1,4) matrix element of the Mueller matrix, as discussed by Bohren and Huffman (12,13). A procedure to obtain all of 16 elements of the (4x4) Mueller matrix, 9 elements simultaneously, is presently being implemented by one of the authors (AHC). These calculated spectra assists AHC in his scattering measurements from sugar and sugar-like compounds. Since the techniques of computational chemistry are now cheaper and faster than extensive experimental techniques, quantum chemistry is used to identify spectral regions of interest in compounds that can be detected by VCD.

This report is organized in the following sections: section II is a background section on VCD in general, the Stephens' formulation of the rotational strength of a vibrational transition and the concept of a Mueller matrix; section III focuses on the 6 carbon sugar molecules that were investigated; section IV is a section which briefly summarizes the current status of scaling of the force field of a molecule and the relation of the scaled force field to VCD parameters for sugars; and section V is a brief summary of this effort.

2. BACKGROUND

Vibrational Circular Dichroism

Molecules that interact differently with left circularly polarized (LCP) and right circularly polarized (RCP) radiation are optically active. Two phenomena linked to optical activity are:

(1) optical rotation
(2) circular dichroism

Optical rotation involves the rotation of a plane of linearly polarized radiation as it is passed through a sample. Circular dichroism is the difference in the absorption of LCP and RCP radiation by a sample. In the absence of applied fields optical activity arises from chirality, which exists when a molecule cannot be superimposed onto its mirror image - i.e., a molecule must not possess any elements of symmetry to be optically active.

In the early 1970's instrumentation was devised to measure the VCD spectrum of a chiral molecule. Here, the difference in absorptivity of a sample between LCP and RCP radiation is plotted as a function of wavenumber. A rotational strength, which corresponds to a difference in absorptivity of a sample between LCP and RCP radiation, can be positive or negative and the intensities are not related to the infrared and Raman intensities. The

essential points to be studied in this investigation are frequencies, magnitudes of intensities and signs of intensities.

Stephens' Formulation of the Rotational Strength

P. J. Stephens (3,4) has developed a theory for the determination of the rotational strength of a vibrational transition g→ e, R(g→ e), for a chiral molecule

$$R(g \to e) = \sum_{\beta} \text{Im}[<g \mid (\mu_{el})_{\beta} \mid e><e \mid (\mu_{mag})_{\beta} \mid g>] \qquad [\beta = x, y, z] \qquad (1)$$

where g and e are ground and excited states and μ_{el} and μ_{mag} are electric and magnetic dipole moment operators. For a *given* fundamental vibrational mode of frequency ω_i, the electric and magnetic dipole transition moments for the 0→ 1 vibrational transition is given by

$$<o \mid (\mu_{el})_{\beta} \mid 1>_i = (h / 2\omega_i)^{1/2} \sum_{\lambda\alpha} P_{\alpha\beta}^{\lambda} \, S_{\lambda\alpha,i} \qquad (2)$$

$$<o \mid (\mu_{mag})_{\beta} \mid 1>_i = - (2h^3\omega_i)^{1/2} \sum_{\lambda\alpha} M_{\alpha\beta}^{\lambda} \, S_{\lambda\alpha,i}. \qquad (3)$$

$P_{\alpha\beta}^{\lambda}$ and $M_{\alpha\beta}^{\lambda}$ are atomic polar and atomic axial tensors defined by

$$P_{\alpha\beta}^{\lambda} = E_{\alpha\beta}^{\lambda} + N_{\alpha\beta}^{\lambda} \qquad (4)$$

$$M_{\alpha\beta}^{\lambda} = I_{\alpha\beta}^{\lambda} + J_{\alpha\beta}^{\lambda} \qquad (5)$$

$$E_{\alpha\beta}^{\lambda} = [(\partial/\partial X_{\lambda\alpha}) <\psi_G(\vec{R}) \mid (\mu_{el}^e)_{\beta} \mid \psi_G(\vec{R})>]_{R_o} \qquad (6)$$

$$N_{\alpha\beta}^{\lambda} = Z_{\lambda}e\delta_{\alpha\beta} \qquad (7)$$

$$I_{\alpha\beta}^{\lambda} = <(\partial\psi_G(\vec{R})/\partial X_{\lambda\alpha})_{R_o} \mid (\partial\psi_G(\vec{R}_o, H_\beta)/\partial H_\beta)_{H_o=0}> \qquad (8)$$

$$J_{\alpha\beta}^{\lambda} = (i / 4hc) \sum_{\gamma} \epsilon_{\alpha\beta\gamma}(Z_{\lambda}e)R_{\lambda\gamma}^o \qquad (9)$$

where

$\vec{R}$ = the nuclear geometry,

$\vec{R}_0$ = the equilibrium nuclear geometry,

$X_{\lambda\alpha}$ = cartesian displacement coordinates (α = x,y,z) from equilibrium of nucleus λ,

Z_{λ} e = charge on nucleus λ,

$\vec{R}_\lambda^0$ = equilibrium position of nucleus λ,

G = electronic ground state,

μ_{el}^e = electronic contribution to μ_{el},

$\psi_G(\vec{R}_0, H_\beta)$ = electronic wavefunction of G at $\vec{R}_0$ in the presence of the perturbation
$H = -(\mu_{mag}^e)_\beta H_\beta$, and

$\epsilon_{\alpha\beta\gamma}$ = antisymmetric unit third rank tensor.

Note that

$$X_{\lambda\alpha} = \sum_i S_{\lambda\alpha,i} Q_i$$

i.e. $S_{\lambda\alpha,i}$ is a matrix element in the transformation between the cartesian coordinates and the normal coordinates.

Mueller Matrix

Let us now turn to a brief discussion of the definition and use of a Mueller matrix. First let us consider the transmission of electromagnetic radiation. The interaction of polarized radiation with an optical element (polarizer, retarder, reflector, scatterer) can be described by specifying the polarization state of incident and transmitted radiation. One convenient description of the radiation involves use of Stokes vectors and the use of a transformation between the transmitted radiation, σ_t, and the incident radiation, σ_i, which is termed the Mueller matrix (12,13), **T**.

$$\sigma_t = \mathbf{T}\sigma_i \qquad (10)$$

All of the information concerning the transmission of radiation by an optical element is contained in the 16 elements of the transformation Mueller matrix. The Stokes parameters (I,Q,U,V), components of a Stokes vector (σ), are defined by

$$\sigma = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}$$

$$I = <|\hat{\epsilon}_1 \cdot E|^2> + <|\hat{\epsilon}_2 \cdot E|^2> \qquad (11)$$

$$Q = <|\hat{\epsilon}_1 \cdot E|^2> - <|\hat{\epsilon}_2 \cdot E|^2> \qquad (12)$$

$$U = <2Re(\hat{\epsilon}_1 \cdot E)(\hat{\epsilon}_2 \cdot E)> \qquad (13)$$

$$V = <2Im(\hat{\epsilon}_1 \cdot E)(\hat{\epsilon}_2 \cdot E)> \qquad (14)$$

where elements of the Stokes column matrix are defined in terms of the unit orthogonal coordinate basis vectors $\hat{\epsilon}_{1,2}$, and the angular brackets indicate a time average over an interval long compared with the period of a quasi-monochromatic beam described by an electric field.

Now, if scattered radiation from a single particle or a collection of particles is studied, an analogous Mueller matrix for scattering (14), S, can be setup.

$$\sigma_s = S\sigma_i \tag{15}$$

If the incident light is right-circularly polarized, then the irradiance I_R of the scattered light is $S_{11} + S_{14}$. Also, the irradiance I_L of the scattered light is $S_{11} - S_{14}$. The Mueller scattering matrix element S_{14} can be expressed as

$$S_{14} = (I_R - I_L)/2I_i \tag{16}$$

where I_i is the intensity of the incident light. The matrix element S_{14} is readily interpretable in terms of the difference of the irradiances of scattered light for incident right-circularly and left-circularly polarized light. The VCD intensity is directly proportional to the S_{14} matrix element, and therefore, a VCD theoretical spectrum can be used to predict the magnitude of the Mueller matrix element S_{14}.

3. SUGAR MOLECULES INVESTIGATED

The task undertaken on this project was the prediction of the vibrational circular dichroism spectra (VCD) of the D enantiomers of the hexoses (sugars with 6 carbon atoms). There are 8 such sugar molecules with molecular formula $C_6H_{12}O_6$: aldose, altrose, glucose, mannose, idose, gulose, talose, and galactose. In this report we have considered these molecules only in a linear configuration. Studies on the cyclic forms of these sugars will follow. The calculations have proceeded in the following stepwise manner:

(1) based on previous geometries of 5 carbon sugars a reasonable starting geometry of D-allose was obtained and used in an optimization using the Gaussian 90 (17-20) electronic structure program.

(2) frequencies and rotational strengths were obtained by running CADPAC version 4.2 (21).

(3) by suitable change of dihedral angles starting geometries were devised for the other D-enantiomers. Steps (1) and (2) were repeated for each of the 8 D-enantiomers of the hexoses.

The calculations on the sugars have been carried out at the 3-21G level. This level was selected because past experience indicates very reasonable optimized structures are found as compared to experimental structures. As is well known with ab initio determination of vibrational motion, the vibrational frequencies are typically too high by roughly 10 per cent - e.g. the C-H stretch predicted for 3-21 G level calculations multiplied by a scaling factor of 0.89, found empirically, gives very good agreement with experimental observations. (22,23)

In this work:

(1) the optimized geometry at the 3-21G level of calculation of 7 of the 8 D-hexoses have been determined; the optimization of galactose is in progress and

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(2) the prediction of VCD spectral parameters, wavenumbers and rotational strengths for 6 of the 8 hexoses (vide supra) have been determined; in progress are calculations on D-gulose and D-galactose.

Our objectives are:

(1) develop the VCD parameters (frequency and rotational strengths) in the range 800-1200 cm^{-1} that indicate transitions of high rotational strength and predict the correct sign.

(2) develop the VCD parameters as accurately as possible, within a procedure that is computationally reasonable, for sugars in order that the results can be dovetailed into the experimental program on Mueller Matrix Spectroscopy directed by one of the authors (AHC).

Attention was focused on sugar molecules with six carbon atoms (23). The calculated frequencies, rotational strengths and optimized geometries for the molecular predictions completed in this task are reported in Tables 1-16 and the optimized geometries are shown in Figures 1-8.

Through examination of given spectral ranges it is possible to scan each table of frequencies and rotational strengths to predict the frequency a maximum rotational strength should be observed. The quality of the results can be seen by focusing on the VCD parameters reported in Tables 2, 4, 6, 8, 10, 12, 14, and 16. The key points to note are:

(1) The calculation is sensitive, because of the nature of the quantum mechanical operators involved (viz, the angular momentum), to the choice of origin of the coordinate system. Comparisons in the literature at present find better agreement with the choice of origin as the center of mass of the molecule. Key to the calculation is the level of the calculation. As mentioned earlier, our calculations are carried out at the 3-21G level, the origin chosen was the center of mass. The gauge origin used is the distributed origin, following the recommendation of Stephens.

(2) The inaccuracies that result will be manifest in

- force field generated
- atomic polar tensor
- atomic axial tensor

It is appropriate to point out that the size of the basis set for a 3-21G level of calculation is given by 22 n, where n corresponds to the molecular formula $(CH_2O)_n$. For the hexoses the basis set size is 132, which is a fairly large basis set by today's standards. Note that the ab initio unscaled frequencies will be somewhat high (roughly about 10 %) compared to experimental frequencies.

The following work is suggested to continue the project toward the generation of a library of theoretically predicted VCD spectra:

(1) Investigate the hexoses in ring configurations.

(2) Label the modes of vibration for all molecules that were studied and compare with experimental data or other calculations where available.

(3) Investigate the use of scaled force field and their effects on calculated

frequencies, atomic polar and atomic axial tensors and their subsequent effect on rotational strengths.

(4) Investigate larger basis set calculations, such as 6-31G or 6-31G*, using the 3-21G optimized structures as starting geometries.

In order to obtain quantitative accuracy in the prediction of the VCD spectrum of a molecule, some form of scaling is definitely needed. However, if the main intent of the calculations is to predict the transitions of high rotational strength and their correct signs, then 3-21G seems to be an adequate level to do the calculations based on the small set of molecules that have been studied.

4. SCALING OF FORCE FIELD

We have performed some preliminary studies in preparation for scaling of the force field of a molecule in order to obtain more realistic VCD parameter for sugars. The following tasks have been started and are in progress:

(1) a QCPE program has been used to obtain the transformation matrix, B, between internal coordinates and cartesian coordinates,

(2) scaling of the diagonal elements of the force constant matrix for methyl thiirane has reproduced results in the literature,

(3) a set of 8 molecules with functionalities common to sugars have been optimized as a step in preparation for developing scaling parameters for various internal motion,

(4) it is planned to compare the scaling constants obtained for small molecules, with the expectation of transferal from molecule to molecule, to the constants which optimize agreement with experimental frequencies of a molecule and all known isotopomers.

(5) a scaled force constant matrix has been derived from the B transformation matrix and the unscaled force constant matrix, and

(6) a procedure has been devised to incorporate the scaled force constant matrix into CADPAC for the purpose of determining normal mode frequencies and intensities.

5. SUMMARY

This study represents continuing work toward the goal of generating theoretically predicted VCD spectra of sugars. The approach involves the use of Stephens' theoretical formulation of the rotational strength and the use of Gaussian calculations at the 3-21G level of calculation. It should be emphasized that the key assumptions being used are:

(1) use of Stephens' theoretical formulation

(2) use of Gaussian 3-21G level of calculation

The level of calculation affects the frequencies, atomic polar tensor, atomic axial tensor, and thereby the rotational strength.

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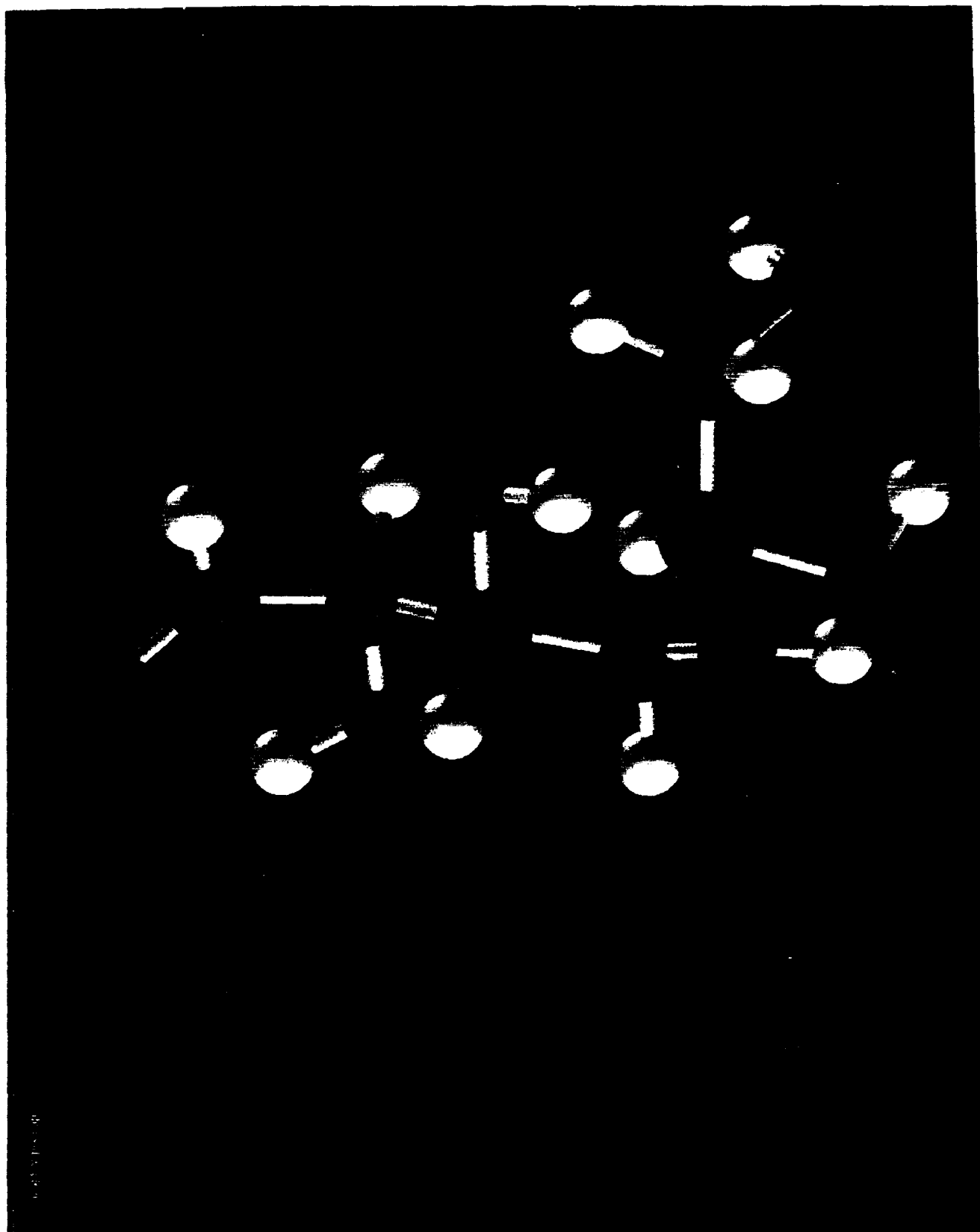
Figure 1. Optimized geometry for D-Allose
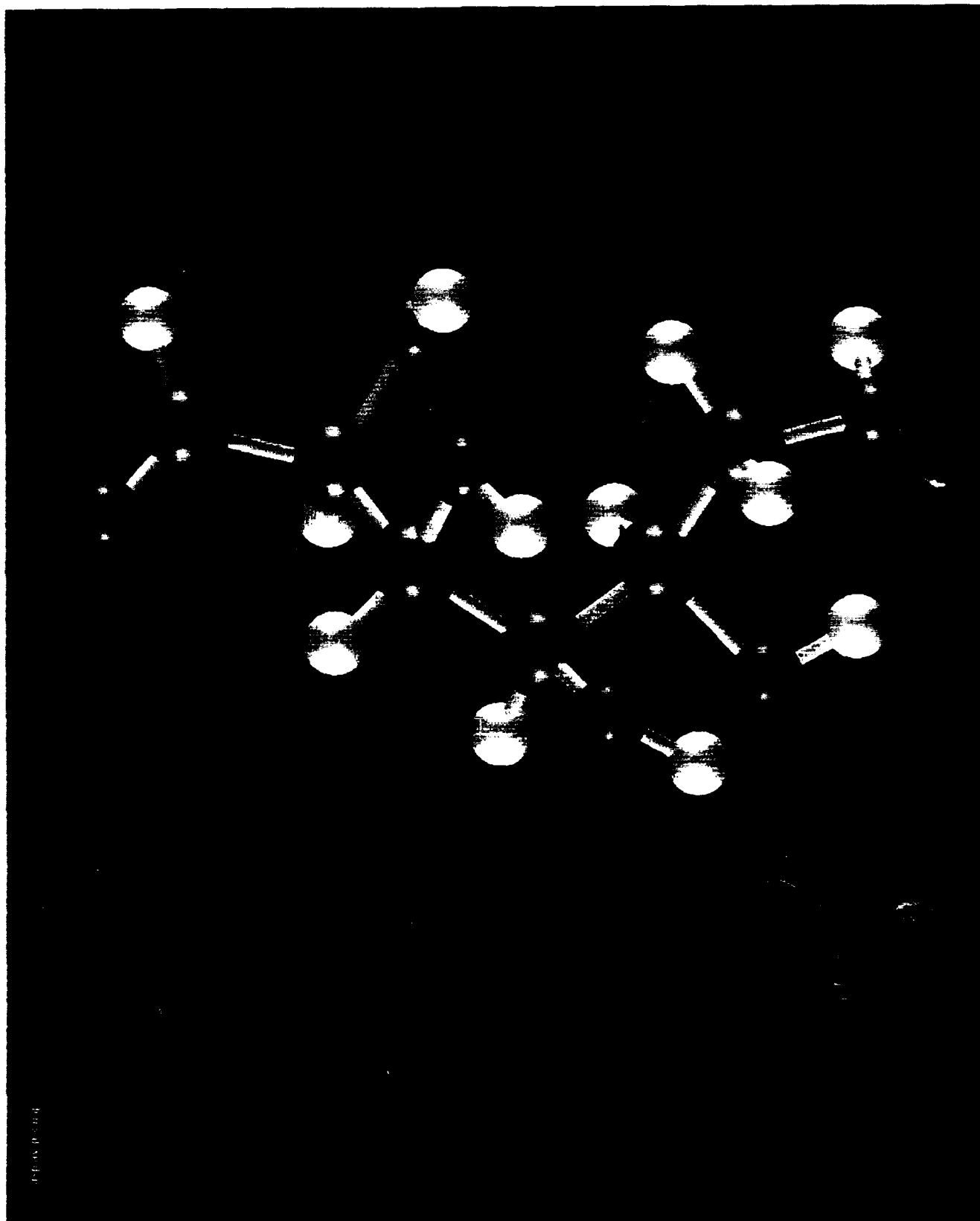
Figure 2. Optimized geometry for D-Altrose
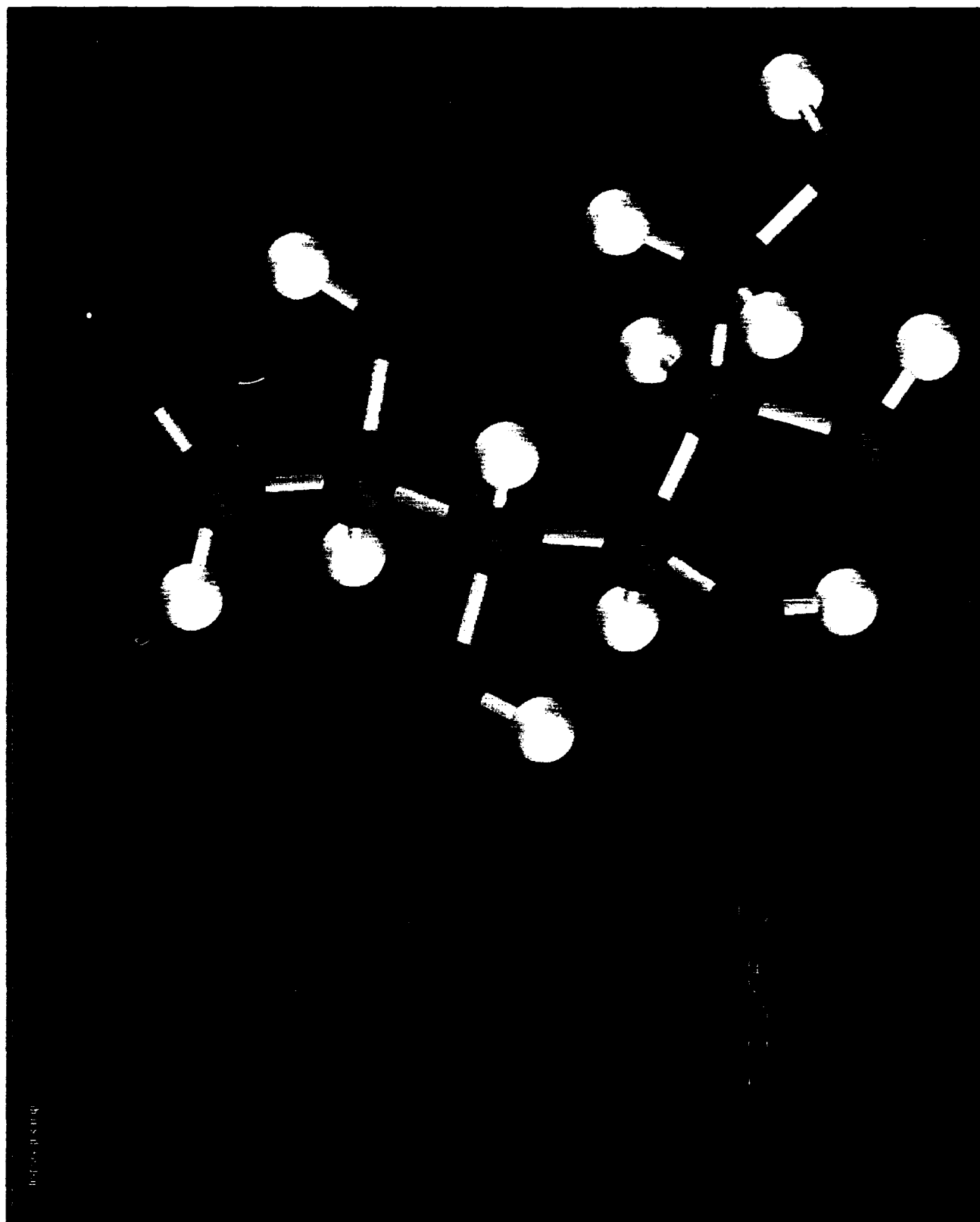
Figure 3. Optimized geometry for D-Mannose
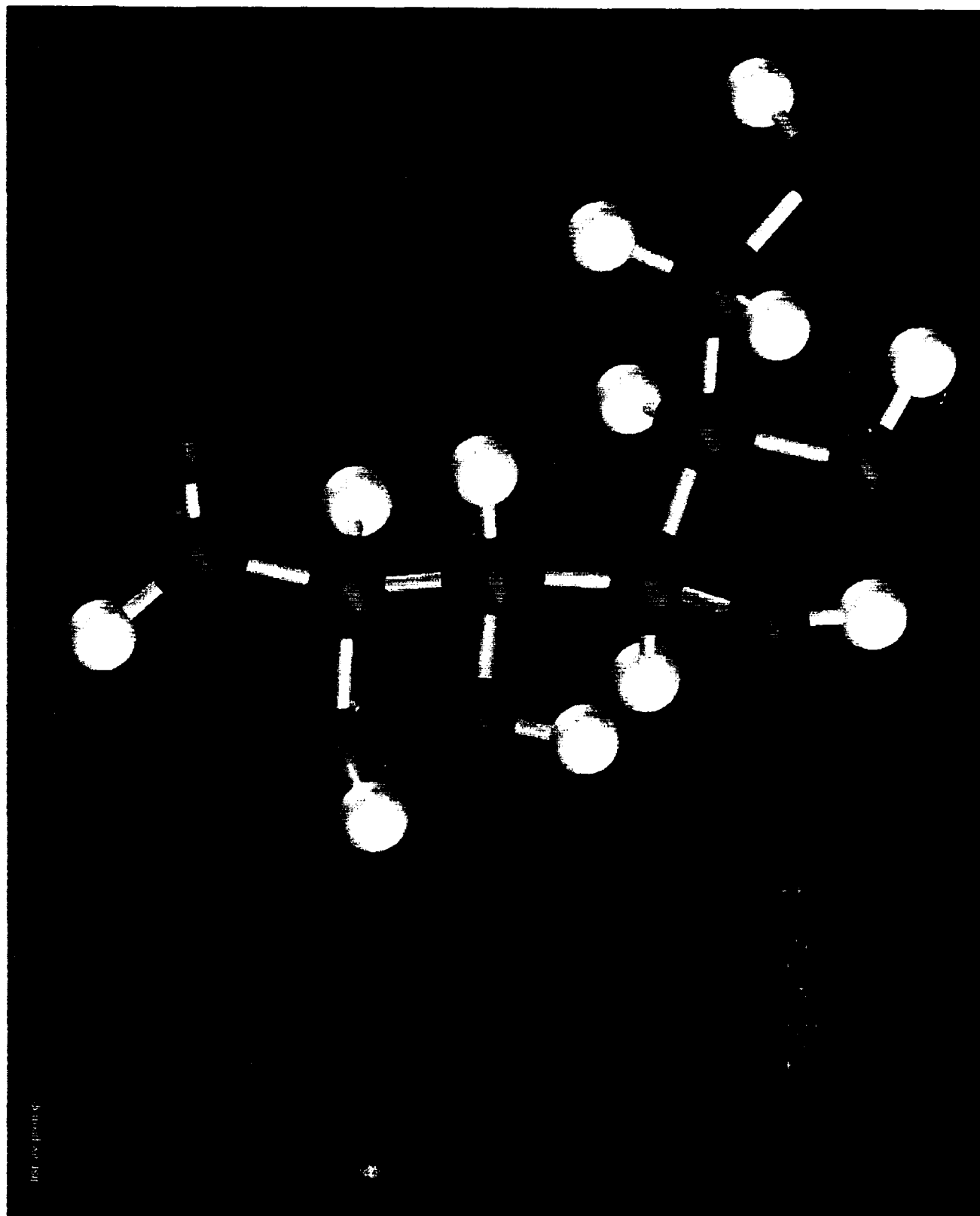
Figure 4. Optimized geometry for D-Glucose
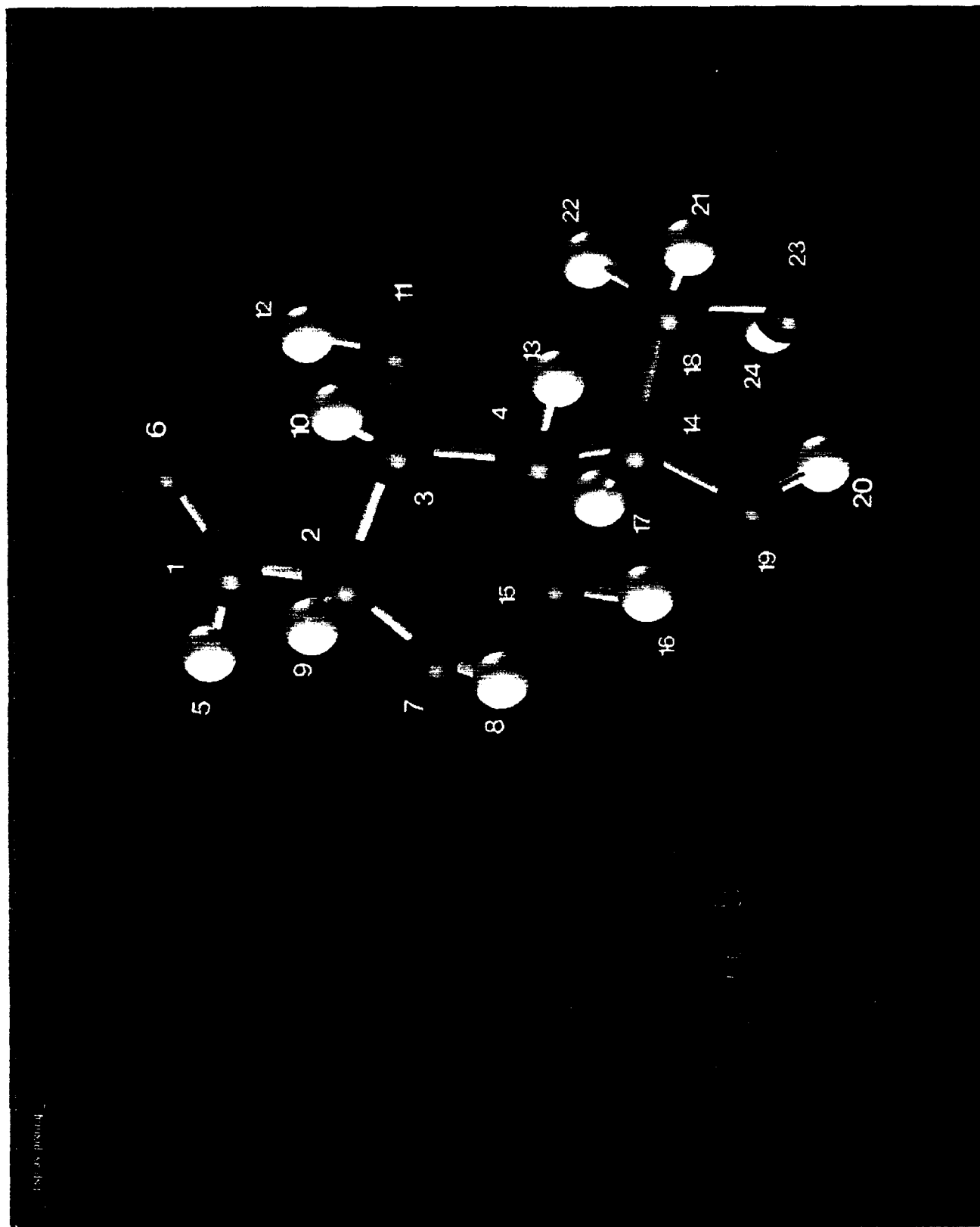
Figure 5. Optimized geometry for D-Idose
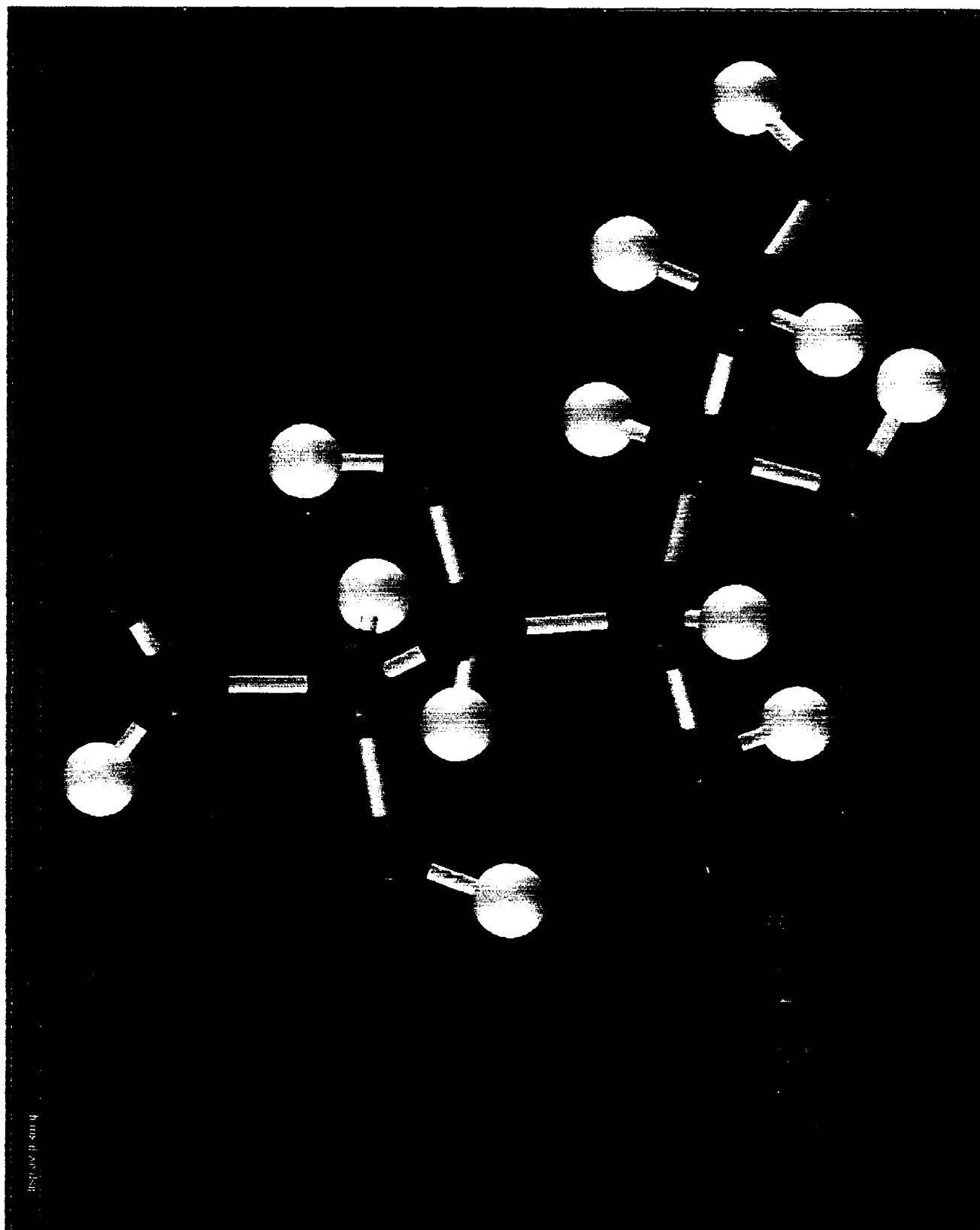
Figure 6. Optimized geometry for D-Gulose
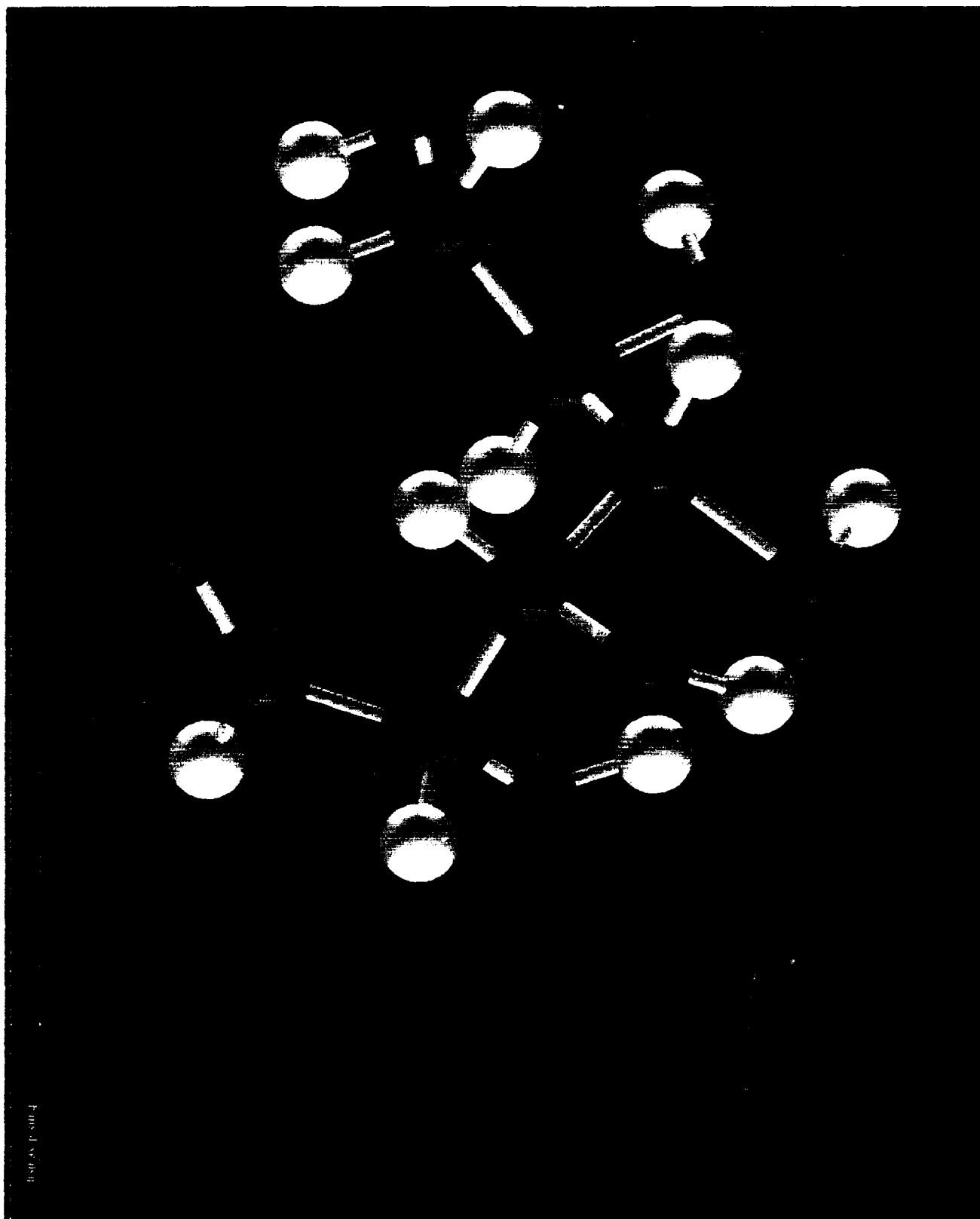
Figure 7. Optimized geometry for D-Talose
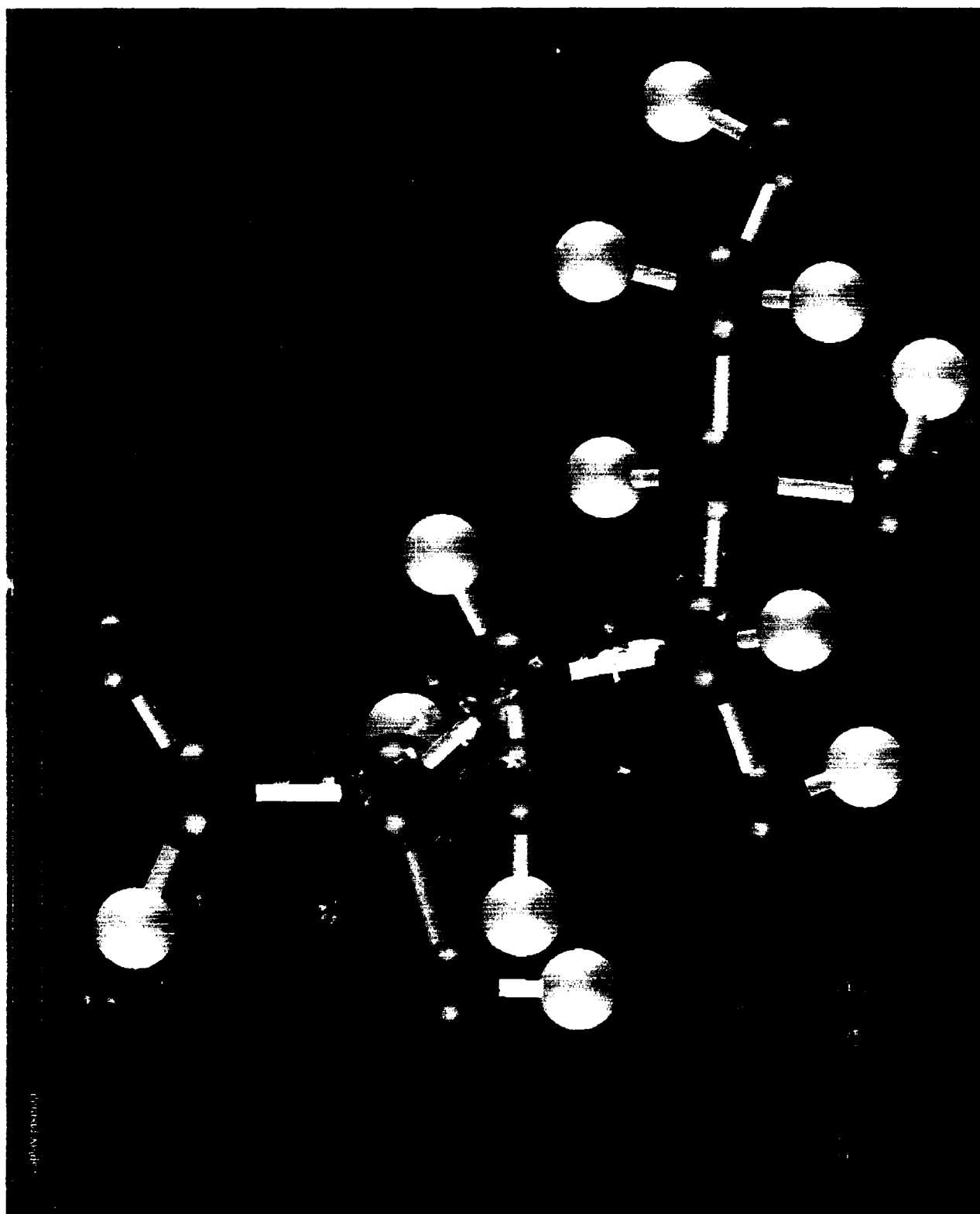
Figure 8. Optimized geometry for D-Galactose

Table 1. Optimized Geometry for D-Allose [CHO-HCOH-HCOH-HCOH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.532701306 a.u. and the dipole moment = 2.133612 D.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5087
$r(C_2\text{-}C_3)$	1.5203 A
$r(C_3\text{-}C_4)$	1.5178 A
$r(C_1\text{-}H_5)$	1.0789 A
$r(C_1\text{-}O_6)$	1.2113 A
$r(C_2\text{-}O_7)$	1.4242 A
$r(C_2\text{-}H_8)$	1.0827 A
$r(O_7\text{-}H_9)$	0.9710 A
$r(C_3\text{-}H_{10})$	1.0837 A
$r(C_3\text{-}O_{11})$	1.4346 A
$r(O_{11}\text{-}H_{12})$	0.9690 A
$r(C_4\text{-}H_{13})$	1.0785 A
$r(C_4\text{-}C_{14})$	1.5210 A
$r(C_4\text{-}O_{15})$	1.4440 A
$r(O_{15}\text{-}H_{16})$	0.9692 A
$r(C_{14}\text{-}H_{17})$	1.0823 A
$r(C_{14}\text{-}C_{18})$	1.5265 A
$r(C_{14}\text{-}O_{19})$	1.4481 A
$r(O_{19}\text{-}H_{20})$	0.9699 A
$r(C_{18}\text{-}H_{21})$	1.0765 A
$r(C_{18}\text{-}H_{22})$	1.0746 A
$r(C_{18}\text{-}H_{23})$	1.4550 A
$r(O_{23}\text{-}H_{24})$	0.9661 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	109.237 °
$\phi(C_4\text{-}C_3\text{-}C_2)$	113.625 °
$\phi(H_5\text{-}C_1\text{-}C_2)$	115.307 °
$\phi(O_6\text{-}C_1\text{-}C_2)$	121.147 °
$\phi(O_7\text{-}C_2\text{-}C_3)$	109.212 °
$\phi(H_8\text{-}C_2\text{-}C_3)$	108.660 °
$\phi(H_9\text{-}O_7\text{-}C_2)$	108.955 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	109.622 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	105.202 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	107.646 °
$\phi(H_{13}\text{-}C_4\text{-}C_3)$	109.240 °
$\phi(C_{14}\text{-}C_4\text{-}C_3)$	116.579 °
$\phi(O_{15}\text{-}C_4\text{-}C_3)$	103.778 °

Table 1. Optimized Geometry for D-Allose [CHO-HCOH-HCOH-HCOH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.532701306 a.u. and the dipole moment = 2.133612 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	107.042 °
$\phi(H_{17}\text{-}C_{14}\text{-}C_4)$	110.141 °
$\phi(C_{18}\text{-}C_{14}\text{-}C_4)$	114.774 °
$\phi(O_{19}\text{-}C_{14}\text{-}C_4)$	103.205 °
$\phi(H_{20}\text{-}O_{19}\text{-}C_{14})$	107.269 °
$\phi(H_{21}\text{-}C_{18}\text{-}C_{14})$	113.183 °
$\phi(H_{22}\text{-}C_{18}\text{-}C_{14})$	108.938 °
$\phi(H_{23}\text{-}C_{18}\text{-}C_{14})$	107.111 °
$\phi(H_{24}\text{-}O_{23}\text{-}C_{14})$	104.193 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	171.203 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	55.100 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	-124.325 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	50.484 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	-71.004 °
$\tau(H_9\text{-}O_7\text{-}C_2\text{-}C_1)$	4.007 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	51.127 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	-67.836 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	187.321 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-71.560 °
$\tau(C_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	51.078 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	-190.447 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	187.696 °
$\tau(H_{17}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-69.166 °
$\tau(C_{18}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	57.433 °
$\tau(O_{19}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-187.465 °
$\tau(H_{20}\text{-}O_{19}\text{-}C_{14}\text{-}C_4)$	200.976 °
$\tau(H_{21}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-72.454 °
$\tau(H_{22}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	49.312 °
$\tau(H_{23}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-196.623 °
$\tau(H_{24}\text{-}O_{23}\text{-}C_{14}\text{-}C_4)$	224.575 °

Table 2. Calculated Wavenumbers $\hat{\nu}$ and Rotational Strengths R for D-Allose [CHO-HCOH-HCOH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry.

$\hat{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
52.59	14.710
64.85	-16.555
103.06	18.665
143.19	-39.354
158.54	18.545
167.54	-8.769
210.28	44.743
263.56	17.824
292.37	11.132
311.20	60.635
320.94	-88.576
334.37	-7.591
352.29	-20.802
367.38	-1.531
455.12	-29.528
460.35	-71.927
522.69	90.392
554.17	80.522
590.32	11.152
602.16	59.302
654.85	-38.471
692.47	-75.077
802.00	-38.208
827.93	-51.259
890.53	-15.821
928.25	-14.187
964.86	131.950
1037.10	-37.785
1089.92	163.110
1110.71	-235.750
1129.18	-15.280
1141.91	81.167
1162.17	-17.818
1188.22	89.104
1204.47	-119.73
1246.31	-25.781
1288.53	-19.950
1354.50	152.130
1364.71	40.903
1391.41	104.280
1398.47	-90.794

Table 2. Calculated Wavenumbers $\dot{\nu}$ and Rotational Strengths R for D-Allose [CHO-HCOH-HCOH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry. (Continued)

$\dot{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
1439.73	-55.255
1453.75	-48.573
1483.17	30.799
1500.26	-18.187
1506.69	5.050
1512.44	-18.719
1518.71	-0.882
1525.40	17.372
1572.11	-8.048
1578.42	26.216
1587.42	24.669
1669.45	3.816
1903.68	0.068
3217.48	14.326
3236.11	-52.773
3243.74	41.509
3278.94	-2.267
3293.21	-2.952
3297.96	-9.403
3360.94	6.792
3821.55	5.886
3844.74	5.269
3862.83	3.909
3865.66	-4.044
3875.82	1.918

Table 3. Optimized Geometry for D-Altrose [CHO-HOCH-HCOH-HCOH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.533109440 a.u. and the dipole moment = 2.558607 D.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5169 A
$r(C_2\text{-}C_3)$	1.5232 A
$r(C_3\text{-}C_4)$	1.5165 A
$r(C_1\text{-}H_5)$	1.0843 A
$r(C_1\text{-}O_6)$	1.2068 A
$r(C_2\text{-}O_7)$	1.4327 A
$r(C_2\text{-}H_8)$	1.0826 A
$r(O_7\text{-}H_9)$	0.9702 A
$r(C_3\text{-}H_{10})$	1.0795 A
$r(C_3\text{-}O_{11})$	1.4423 A
$r(O_{11}\text{-}H_{12})$	0.9681 A
$r(C_4\text{-}H_{13})$	1.0830 A
$r(C_4\text{-}C_{14})$	1.5226 A
$r(C_4\text{-}O_{15})$	1.4426 A
$r(O_{15}\text{-}H_{16})$	0.9693 A
$r(C_{14}\text{-}H_{17})$	1.0813 A
$r(C_{14}\text{-}C_{18})$	1.5252 A
$r(C_{14}\text{-}O_{19})$	1.4486 A
$r(O_{19}\text{-}H_{20})$	0.9702 A
$r(C_{18}\text{-}H_{21})$	1.0721 A
$r(C_{18}\text{-}H_{22})$	1.0745 A
$r(C_{18}\text{-}H_{23})$	1.4552 A
$r(O_{23}\text{-}H_{24})$	0.9662 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	110.647 °
$\phi(C_4\text{-}C_3\text{-}C_2)$	114.960 °
$\phi(H_5\text{-}C_1\text{-}C_2)$	113.332 °
$\phi(O_6\text{-}C_1\text{-}C_2)$	123.596 °
$\phi(O_7\text{-}C_2\text{-}C_3)$	110.789 °
$\phi(H_8\text{-}C_2\text{-}C_3)$	110.870 °
$\phi(H_9\text{-}O_7\text{-}C_2)$	106.159 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	108.870 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	104.470 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	108.101 °
$\phi(H_{13}\text{-}C_4\text{-}C_3)$	109.151 °
$\phi(C_{14}\text{-}C_4\text{-}C_3)$	117.686 °
$\phi(O_{15}\text{-}C_4\text{-}C_3)$	104.175 °

Table 3. Optimized Geometry for D-Altrose [CHO-HOCH-HCOH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level of Calculation. [The total energy = -679.533109440 a.u. and the dipole moment = 2.558607 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}-O_{15}-C_4)$	107.138 °
$\phi(H_{17}-C_{14}-C_4)$	111.054 °
$\phi(C_{18}-C_{14}-C_4)$	115.187 °
$\phi(O_{19}-C_{14}-C_4)$	102.578 °
$\phi(H_{20}-O_{19}-C_{14})$	107.080 °
$\phi(H_{21}-C_{18}-C_{14})$	111.575 °
$\phi(H_{22}-C_{18}-C_{14})$	109.668 °
$\phi(H_{23}-C_{18}-C_{14})$	107.005 °
$\phi(H_{24}-O_{23}-C_{14})$	105.092 °
$\tau(C_4-C_3-C_2-C_1)$	159.096 °
$\tau(H_5-C_1-C_2-C_3)$	144.312 °
$\tau(O_6-C_1-C_2-C_3)$	-36.632 °
$\tau(O_7-C_2-C_3-C_4)$	279.616 °
$\tau(H_8-C_2-C_3-C_4)$	38.869 °
$\tau(H_9-O_7-C_2-C_1)$	78.287 °
$\tau(H_{10}-C_3-C_2-C_1)$	37.297 °
$\tau(O_{11}-C_3-C_2-C_1)$	-80.768 °
$\tau(H_{12}-O_{11}-C_3-C_2)$	184.576 °
$\tau(H_{13}-C_4-C_3-C_2)$	-71.159 °
$\tau(C_{14}-C_4-C_3-C_2)$	51.344 °
$\tau(O_{15}-C_4-C_3-C_2)$	-189.286 °
$\tau(H_{16}-O_{15}-C_4-C_3)$	185.695 °
$\tau(H_{17}-C_{14}-C_4-C_3)$	-64.853 °
$\tau(C_{18}-C_{14}-C_4-C_3)$	61.157 °
$\tau(O_{19}-C_{14}-C_4-C_3)$	-183.601 °
$\tau(H_{20}-O_{19}-C_{14}-C_4)$	202.311 °
$\tau(H_{21}-C_{18}-C_{14}-C_4)$	-76.715 °
$\tau(H_{22}-C_{18}-C_{14}-C_4)$	46.054 °
$\tau(H_{23}-C_{18}-C_{14}-C_4)$	-199.284 °
$\tau(H_{24}-O_{23}-C_{14}-C_4)$	221.563 °

Table 4. Calculated Wavenumbers $\dot{\nu}$ and Rotational Strengths R for D-Altrose [CHO-HOCH-HCOH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry.

$\dot{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
45.96	-11.163
93.95	15.105
96.80	2.556
136.91	-68.561
143.59	28.797
173.26	5.195
206.31	34.323
236.42	11.444
282.84	24.365
310.79	54.408
322.37	25.804
331.36	-117.930
343.30	63.508
393.60	-51.834
482.29	39.390
526.03	22.382
561.16	-79.881
600.00	75.989
608.65	-11.358
649.18	-93.884
689.60	44.596
704.81	-46.726
717.24	12.841
837.07	36.120
878.54	50.505
927.86	151.250
989.90	46.704
1041.41	-15.949
1076.84	-182.020
1106.57	34.255
1126.93	-19.696
1142.41	-12.230
1165.39	25.875
1166.34	-78.125
1191.65	-87.410
1224.81	-33.480
1286.11	1.338
1299.35	48.297
1364.31	67.074
1400.19	19.035

Table 4. Calculated Wavenumbers $\bar{\nu}$ and Rotational Strengths R for D-Altrose [CHO-HOCH-HCOH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry. (Continued)

$\bar{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
1426.58	27.454
1431.06	3.548
1469.06	0.116
1485.70	4.464
1496.86	-2.795
1504.49	-11.401
1510.07	12.936
1518.77	22.132
1533.63	-127.360
1556.41	69.948
1574.36	4.909
1589.90	18.354
1666.59	1.222
1921.19	-21.538
3205.56	-3.470
3228.17	16.709
3247.63	17.891
3253.56	-19.517
3285.91	2.008
3323.78	-1.112
3394.94	0.477
3838.21	-250.180
3838.74	252.950
3861.86	0.423
3877.88	-3.052
3882.38	4.017

Table 5. Optimized Geometry for D-Mannose [CHO-HOCH-HOCH-HCOH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.536583009 a.u. and the dipole moment = 1.213027 D.]

geometrical coordinate	value of geometrical coordinate
$r(C_1\text{-}C_2)$	1.5110 A
$r(C_2\text{-}C_3)$	1.5175 A
$r(C_3\text{-}C_4)$	1.5177 A
$r(C_1\text{-}H_5)$	1.0763 A
$r(C_1\text{-}O_6)$	1.2125 A
$r(C_2\text{-}O_7)$	1.4310 A
$r(C_2\text{-}H_8)$	1.0842 A
$r(O_7\text{-}H_9)$	0.9721 A
$r(C_3\text{-}H_{10})$	1.0814 A
$r(C_3\text{-}O_{11})$	1.4366 A
$r(O_{11}\text{-}H_{12})$	0.9691 A
$r(C_4\text{-}H_{13})$	1.0833 A
$r(C_4\text{-}C_{14})$	1.5208 A
$r(C_4\text{-}O_{15})$	1.4428 A
$r(O_{15}\text{-}H_{16})$	0.9700 A
$r(C_{14}\text{-}H_{17})$	1.0781 A
$r(C_{14}\text{-}C_{18})$	1.5239 A
$r(C_{14}\text{-}O_{19})$	1.4480 A
$r(O_{19}\text{-}H_{20})$	0.9702 A
$r(C_{18}\text{-}H_{21})$	1.0777 A
$r(C_{18}\text{-}H_{22})$	1.0771 A
$r(C_{18}\text{-}H_{23})$	1.4539 A
$r(O_{23}\text{-}H_{24})$	0.9663 A
$\phi(C_3\text{-}C_2\text{-}C_1)$	109.866 °
$\phi(C_4\text{-}C_3\text{-}C_2)$	113.352 °
$\phi(H_5\text{-}C_1\text{-}C_2)$	115.750 °
$\phi(O_6\text{-}C_1\text{-}C_2)$	120.556 °
$\phi(O_7\text{-}C_2\text{-}C_3)$	108.868 °
$\phi(H_8\text{-}C_2\text{-}C_3)$	108.800 °
$\phi(H_9\text{-}O_7\text{-}C_2)$	108.266 °
$\phi(H_{10}\text{-}C_3\text{-}C_2)$	109.559 °
$\phi(O_{11}\text{-}C_3\text{-}C_2)$	105.179 °
$\phi(H_{12}\text{-}O_{11}\text{-}C_3)$	107.987 °
$\phi(H_{13}\text{-}C_4\text{-}C_3)$	108.817 °
$\phi(C_{14}\text{-}C_4\text{-}C_3)$	116.890 °
$\phi(O_{15}\text{-}C_4\text{-}C_3)$	103.466 °

Table 5. Optimized Geometry for D-Mannose [CHO-HOCH-HOCH-HCOH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.536583009 a.u. and the dipole moment = 1.213027 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	106.841 °
$\phi(H_{17}\text{-}C_{14}\text{-}C_4)$	110.657 °
$\phi(C_{18}\text{-}C_{14}\text{-}C_4)$	113.615 °
$\phi(O_{19}\text{-}C_{14}\text{-}C_4)$	103.598 °
$\phi(H_{20}\text{-}O_{19}\text{-}C_{14})$	107.067 °
$\phi(H_{21}\text{-}C_{18}\text{-}C_{14})$	110.644 °
$\phi(H_{22}\text{-}C_{18}\text{-}C_{14})$	109.514 °
$\phi(H_{23}\text{-}C_{18}\text{-}C_{14})$	107.599 °
$\phi(H_{24}\text{-}O_{23}\text{-}C_{14})$	104.528 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	173.456 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	305.369 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	125.227 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	292.993 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	54.700 °
$\tau(H_9\text{-}O\text{-}C\text{-}C_1)$	-8.427 °
$\tau(H_{10}\text{-}C\text{-}C_2\text{-}C_1)$	-63.460 °
$\tau(C_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	55.771 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	165.654 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-56.372 °
$\tau(C_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	67.666 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	-173.225 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	191.625 °
$\tau(H_{17}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-73.774 °
$\tau(C_{18}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	50.928 °
$\tau(O_{19}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-193.149 °
$\tau(H_{20}\text{-}O_{19}\text{-}C_{14}\text{-}C_4)$	204.589 °
$\tau(H_{21}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-77.018 °
$\tau(H_{22}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	45.423 °
$\tau(H_{23}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-199.573 °
$\tau(H_{24}\text{-}O_{23}\text{-}C_{14}\text{-}C_4)$	221.737 °

Table 6. Calculated Wavenumbers $\hat{\nu}$ and Rotational Strengths R for D-Mannose [CHO-HOCH-HOCH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry.

$\hat{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
64.12	-6.643
81.11	4.971
115.00	-32.966
126.51	13.936
156.56	7.408
166.34	9.772
212.03	-3.242
276.45	6.573
325.55	49.499
329.57	-126.380
336.31	43.580
344.38	81.699
348.46	-16.551
374.83	4.776
439.32	-14.213
501.77	38.132
537.59	-11.612
559.68	150.470
575.32	-337.240
593.58	-6.336
610.91	123.060
689.47	-54.961
751.72	-103.460
815.33	86.551
917.51	202.800
926.76	-33.473
1011.55	78.480
1070.35	-84.492
1089.85	47.656
1121.97	-19.385
1135.48	4.352
1155.31	-60.527
1176.16	20.371
1182.35	7.573
1199.53	-33.441
1234.23	14.459
1290.98	-29.246
1350.78	32.870
1375.92	10.004
1399.36	10.347

Table 6. Calculated Wavenumbers ν̂ and Rotational Strengths R for D-Mannose [CHO-HOCH-HOCH-HCOH-HCOH-CH₂OH] Based on 3-21G Level Optimized Geometry. (Continued)

ν̂ (cm⁻¹)	R (x 10⁻⁴⁴ esu²cm²)
1406.16	-83.625
1444.61	-11.389
1470.35	-32.723
1482.19	46.612
1490.78	9.943
1499.78	17.461
1500.57	28.490
1512.21	8.019
1523.12	1.218
1559.88	3.073
1588.21	-41.671
1591.80	46.381
1680.16	0.496
1896.38	2.993
3221.35	-2.212
3222.73	14.885
3253.81	5.185
3278.37	-9.021
3291.72	-4.022
3311.11	0.960
3341.58	3.117
3804.80	-15.862
3839.04	21.868
3851.60	-22.410
3864.09	-2.275
3876.29	0.819

Table 7. Optimized Geometry for D-Glucose [CHO-HCOH-HOCH-HCOH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.530797082 a.u. and the dipole moment = 2.8331 D.]

geometrical coordinate	value of geometrical coordinate
$r(C_1-C_2)$	1.5155 A
$r(C_2-C_3)$	1.5236 A
$r(C_3-C_4)$	1.5194 A
$r(C_1-H_5)$	1.0837 A
$r(C_1-O_6)$	1.2079 A
$r(C_2-O_7)$	1.4262 A
$r(C_2-H_8)$	1.0823 A
$r(O_7-H_9)$	0.9716 A
$r(C_3-H_{10})$	1.0785 A
$r(C_3-O_{11})$	1.4432 A
$r(O_{11}-H_{12})$	0.9696 A
$r(C_4-H_{13})$	1.0811 A
$r(C_4-C_{14})$	1.5201 A
$r(C_4-O_{15})$	1.4400 A
$r(O_{15}-H_{16})$	0.9690 A
$r(C_{14}-H_{17})$	1.0834 A
$r(C_{14}-C_{18})$	1.5282 A
$r(C_{14}-O_{19})$	1.4441 A
$r(O_{19}-H_{20})$	0.9704 A
$r(C_{18}-H_{21})$	1.0809 A
$r(C_{18}-H_{22})$	1.0758 A
$r(C_{18}-H_{23})$	1.4524 A
$r(O_{23}-H_{24})$	0.9658 A
$\phi(C_3-C_2-C_1)$	109.812 °
$\phi(C_4-C_3-C_2)$	112.913 °
$\phi(H_5-C_1-C_2)$	113.742 °
$\phi(O_6-C_1-C_2)$	122.915 °
$\phi(O_7-C_2-C_3)$	109.807 °
$\phi(H_8-C_2-C_3)$	111.206 °
$\phi(H_9-O_7-C_2)$	106.180 °
$\phi(H_{10}-C_3-C_2)$	110.175 °
$\phi(O_{11}-C_3-C_2)$	103.264 °
$\phi(H_{12}-O_{11}-C_3)$	107.925 °
$\phi(H_{13}-C_4-C_3)$	108.917 °
$\phi(C_{14}-C_4-C_3)$	116.179 °
$\phi(O_{15}-C_4-C_3)$	104.410 °

Table 7. Optimized Geometry for D-Glucose [CHO-HCOH-HOCH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level of Calculation. [The total energy = -679.530797082 a.u. and the dipole moment = 2.8331 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}-O_{15}-C_4)$	107.444 °
$\phi(H_{17}-C_{14}-C_4)$	111.177 °
$\phi(C_{18}-C_{14}-C_4)$	113.353 °
$\phi(O_{19}-C_{14}-C_4)$	103.606 °
$\phi(H_{20}-O_{19}-C_{14})$	107.329 °
$\phi(H_{21}-C_{18}-C_{14})$	112.526 °
$\phi(H_{22}-C_{18}-C_{14})$	108.714 °
$\phi(H_{23}-C_{18}-C_{14})$	107.489 °
$\phi(H_{24}-O_{23}-C_{14})$	107.453 °
$\tau(C_4-C_3-C_2-C_1)$	189.034 °
$\tau(H_5-C_1-C_2-C_3)$	224.771 °
$\tau(O_6-C_1-C_2-C_3)$	45.763 °
$\tau(O_7-C_2-C_3-C_4)$	68.250 °
$\tau(H_8-C_2-C_3-C_4)$	308.962 °
$\tau(H_9-O_7-C_2-C_1)$	-83.151 °
$\tau(H_{10}-C_3-C_2-C_1)$	-44.803 °
$\tau(O_{11}-C_3-C_2-C_1)$	73.437 °
$\tau(H_{12}-O_{11}-C_3-C_2)$	161.700 °
$\tau(H_{13}-C_4-C_3-C_2)$	-44.595 °
$\tau(C_{14}-C_4-C_3-C_2)$	79.083 °
$\tau(O_{15}-C_4-C_3-C_2)$	-162.454 °
$\tau(H_{16}-O_{15}-C_4-C_3)$	186.454 °
$\tau(H_{17}-C_{14}-C_4-C_3)$	-69.223 °
$\tau(C_{18}-C_{14}-C_4-C_3)$	56.527 °
$\tau(O_{19}-C_{14}-C_4-C_3)$	-188.140 °
$\tau(H_{20}-O_{19}-C_{14}-C_4)$	204.250 °
$\tau(H_{21}-C_{18}-C_{14}-C_4)$	-77.136 °
$\tau(H_{22}-C_{18}-C_{14}-C_4)$	44.688 °
$\tau(H_{23}-C_{18}-C_{14}-C_4)$	-200.311 °
$\tau(H_{24}-O_{23}-C_{14}-C_4)$	223.455 °

Table 8. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for D-Glucose [CHO-HCOH-HOCH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry.

$\tilde{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
50.92	13.317
54.29	-4.002
103.73	-10.132
126.03	20.158
142.11	4.490
159.67	15.775
185.71	19.412
236.33	-13.157
286.51	-1.323
295.20	17.384
322.31	-43.350
352.93	-1.195
355.82	-7.555
411.22	-12.653
490.21	40.281
512.17	-8.987
576.38	18.910
584.70	-43.761
596.40	91.349
662.44	110.510
670.26	-10.941
683.84	-399.150
706.53	150.900
762.67	-104.400
919.00	-2.724
930.56	-124.810
1010.02	43.154
1048.88	116.100
1090.30	108.390
1111.17	-91.097
1120.65	-57.094
1143.57	15.994
1160.68	114.030
1182.46	24.243
1191.69	-36.172
1220.39	30.456
1285.47	-42.736
1307.43	-68.572
1364.71	20.115

Table 8. Calculated Wavenumbers $\bar{\nu}$ and Rotational Strengths R for D-Glucose [CHO-HCOH-HOCH-HCOH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry. (Continued)

$\bar{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
1396.10	48.805
1431.24	-45.148
1445.47	-30.692
1464.56	-7.211
1483.56	32.667
1489.14	62.352
1495.22	4.043
1500.54	-6.535
1518.83	-0.926
1524.53	-50.511
1536.20	69.525
1570.86	35.104
1585.77	-8.738
1679.01	4.663
1914.99	20.760
3211.74	3.148
3216.01	9.510
3247.03	-8.456
3249.08	2.469
3261.71	9.709
3295.03	-14.540
3341.47	4.144
3820.75	-20.644
3836.07	1.302
3858.38	-6.849
3867.61	4.369
3882.34	0.458

Table 9. Optimized Geometry for D-Idose [CHO-HOCH-HCOH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level of Calculation. [The total energy = -679.535466855 a.u. and the dipole moment = 0.090621 D.]

geometrical coordinate	value of geometrical coordinate
r(C$_1$-C$_2$)	1.5059 A
r(C$_2$-C$_3$)	1.5372 A
r(C$_3$-C$_4$)	1.5281 A
r(C$_1$-H$_5$)	1.0820 A
r(C$_1$-O$_6$)	1.2132 A
r(C$_2$-O$_7$)	1.4322 A
r(C$_2$-H$_8$)	1.0853 A
r(O$_7$-H$_9$)	0.9699 A
r(C$_3$-H$_{10}$)	1.0833 A
r(C$_3$-O$_{11}$)	1.4360 A
r(O$_{11}$-H$_{12}$)	0.9676 A
r(C$_4$-H$_{13}$)	1.0827 A
r(C$_4$-C$_{14}$)	1.5299 A
r(C$_4$-O$_{15}$)	1.4469 A
r(O$_{15}$-H$_{16}$)	0.9725 A
r(C$_{14}$-H$_{17}$)	1.0776 A
r(C$_{14}$-C$_{18}$)	1.5221 A
r(C$_{14}$-O$_{19}$)	1.4507 A
r(O$_{19}$-H$_{20}$)	0.9692 A
r(C$_{18}$-H$_{21}$)	1.0736 A
r(C$_{18}$-H$_{22}$)	1.0791 A
r(C$_{18}$-H$_{23}$)	1.4558 A
r(O$_{23}$-H$_{24}$)	0.9661 A
ϕ(C$_3$-C$_2$-C$_1$)	112.429 °
ϕ(C$_4$-C$_3$-C$_2$)	111.253 °
ϕ(H$_5$-C$_1$-C$_2$)	113.320 °
ϕ(O$_6$-C$_1$-C$_2$)	124.315 °
ϕ(O$_7$-C$_2$-C$_3$)	115.251 °
ϕ(H$_8$-C$_2$-C$_3$)	106.845 °
ϕ(H$_9$-O$_7$-C$_2$)	106.279 °
ϕ(H$_{10}$-C$_3$-C$_2$)	106.854 °
ϕ(O$_{11}$-C$_3$-C$_2$)	113.491 °
ϕ(H$_{12}$-O$_{11}$-C$_3$)	109.554 °
ϕ(H$_{13}$-C$_4$-C$_3$)	110.085 °
ϕ(C$_{14}$-C$_4$-C$_3$)	113.135 °
ϕ(O$_{15}$-C$_4$-C$_3$)	107.363 °

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Table 9. Optimized Geometry for D-Idose [CHO-HOCH-HCOH-HOCH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.535466855 a.u. and the dipole moment = 0.090621 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	106.049 °
$\phi(H_{17}\text{-}C_{14}\text{-}C_4)$	109.818 °
$\phi(C_{18}\text{-}C_{14}\text{-}C_4)$	114.563 °
$\phi(O_{19}\text{-}C_{14}\text{-}C_4)$	103.410 °
$\phi(H_{20}\text{-}O_{19}\text{-}C_{14})$	107.579 °
$\phi(H_{21}\text{-}C_{18}\text{-}C_{14})$	111.142 °
$\phi(H_{22}\text{-}C_{18}\text{-}C_{14})$	109.971 °
$\phi(H_{23}\text{-}C_{18}\text{-}C_{14})$	107.320 °
$\phi(H_{24}\text{-}O_{23}\text{-}C_{14})$	104.602 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	202.359 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	163.574 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	-16.821 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	322.103 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	84.728 °
$\tau(H_9\text{-}O_7\text{-}C_2\text{-}C_1)$	-169.024 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	82.875 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	-38.782 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	60.412 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-152.682 °
$\tau(C_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	85.403 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	-33.541 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	165.230 °
$\tau(H_{17}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-41.875 °
$\tau(C_{18}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	84.376 °
$\tau(O_{19}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-159.587 °
$\tau(H_{20}\text{-}O_{19}\text{-}C_{14}\text{-}C_4)$	205.421 °
$\tau(H_{21}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-75.133 °
$\tau(H_{22}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	47.046 °
$\tau(H_{23}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-198.796 °
$\tau(H_{24}\text{-}O_{23}\text{-}C_{14}\text{-}C_4)$	222.334 °

Table 10. Calculated Wavenumbers $\dot{v}$ and Rotational Strengths R for D-Idose [CHO-HOCH-HCOH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry.

$\dot{v}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
61.03	0.999
80.34	4.912
94.91	20.102
123.31	6.433
159.14	4.871
202.38	-20.232
247.85	12.589
254.08	-23.272
287.14	20.792
322.89	-9.871
328.72	-14.110
381.16	-31.964
389.00	17.039
411.63	-35.588
445.86	-29.007
530.96	5.690
560.74	9.015
600.46	48.259
623.87	-96.674
636.18	-78.534
664.05	-129.710
760.08	181.820
764.93	-53.337
795.55	-85.015
834.27	-26.272
966.17	8.267
1018.17	2.945
1033.37	-51.988
1088.38	13.471
1100.05	169.000
1124.77	49.046
1155.17	-17.515
1156.79	89.289
1178.72	-1.952
1191.19	-11.517
1247.20	-70.992
1285.87	-19.892
1363.18	-108.930
1370.87	122.990
1397.21	36.648

Table 10. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for D-Idose [CHO-HOCH-HCOH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry. (Continued)

$\tilde{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
1418.37	24.023
1455.03	-50.734
1465.51	-10.434
1479.52	14.804
1503.28	13.306
1519.45	72.299
1524.04	-59.109
1528.25	-21.254
1547.31	-37.478
1552.48	35.198
1572.92	84.083
1581.28	0.906
1677.07	4.892
1900.21	-22.664
3201.44	-12.812
3221.56	-27.269
3237.13	-9.879
3239.84	29.305
3270.81	-0.971
3305.33	4.920
3369.77	-3.649
3811.06	-17.715
3844.63	-26.632
3854.49	7.810
3867.64	-23.971
3877.52	5.043

Table 11. Optimized Geometry for D-Gulose [CHO-HCOH-HCOH-HOCH-HCOH-CH_2OH] Based on 3-21G Level of Calculation. [The total energy = -679.541445638 a.u. and the dipole moment = 2.3610 D.]

geometrical coordinate	value of geometrical coordinate
$r(C_1-C_2)$	1.5116 A
$r(C_2-C_3)$	1.5342 A
$r(C_3-C_4)$	1.5292 A
$r(C_1-H_5)$	1.0816 A
$r(C_1-O_6)$	1.2148 A
$r(C_2-O_7)$	1.4342 A
$r(C_2-H_8)$	1.0866 A
$r(O_7-H_9)$	0.9752 A
$r(C_3-H_{10})$	1.0832 A
$r(C_3-O_{11})$	1.4348 A
$r(O_{11}-H_{12})$	0.9706 A
$r(C_4-H_{13})$	1.0825 A
$r(C_4-C_{14})$	1.5307 A
$r(C_4-O_{15})$	1.4437 A
$r(O_{15}-H_{16})$	0.9723 A
$r(C_{14}-H_{17})$	1.0814 A
$r(C_{14}-C_{18})$	1.5228 A
$r(C_{14}-O_{19})$	1.4463 A
$r(O_{19}-H_{20})$	0.9694 A
$r(C_{18}-H_{21})$	1.0740 A
$r(C_{18}-H_{22})$	1.0788 A
$r(C_{18}-H_{23})$	1.4546 A
$r(O_{23}-H_{24})$	0.9657 A
$\phi(C_3-C_2-C_1)$	111.029 °
$\phi(C_4-C_3-C_2)$	112.819 °
$\phi(H_5-C_1-C_2)$	113.058 ° °
$\phi(O_6-C_1-C_2)$	124.658 °
$\phi(O_7-C_2-C_3)$	111.915 °
$\phi(H_8-C_2-C_3)$	109.305 °
$\phi(H_9-O_7-C_2)$	107.151 °
$\phi(H_{10}-C_3-C_2)$	107.109 °
$\phi(O_{11}-C_3-C_2)$	110.461 °
$\phi(H_{12}-O_{11}-C_3)$	109.438 °
$\phi(H_{13}-C_4-C_3)$	109.450 °
$\phi(C_{14}-C_4-C_3)$	112.921 °
$\phi(O_{15}-C_4-C_3)$	108.107 °

Table 11. Optimized Geometry for D-Gulose [CHO-HCOH-HCOH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level of Calculation. [The total energy = -679.541445638 a.u. and the dipole moment = 2.3610 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}-O_{15}-C_4)$	106.888 °
$\phi(H_{17}-C_{14}-C_4)$	111..020°
$\phi(C_{18}-C_{14}-C_4)$	114.070 °
$\phi(O_{19}-C_{14}-C_4)$	104.213 °
$\phi(H_{20}-O_{19}-C_{14})$	107.834 °
$\phi(H_{21}-C_{18}-C_{14})$	111.011 °
$\phi(H_{22}-C_{18}-C_{14})$	109.796 °
$\phi(H_{23}-C_{18}-C_{14})$	107.168 °
$\phi(H_{24}-O_{23}-C_{14})$	107.005 °
$\tau(C_4-C_3-C_2-C_1)$	184.356 °
$\tau(H_5-C_1-C_2-C_3)$	212.235 °
$\tau(O_6-C_1-C_2-C_3)$	31.462 °
$\tau(O_7-C_2-C_3-C_4)$	68.825 °
$\tau(H_8-C_2-C_3-C_4)$	303.381 °
$\tau(H_9-O_7-C_2-C_1)$	-169.061 °
$\tau(H_{10}-C_3-C_2-C_1)$	63.940 °
$\tau(O_{11}-C_3-C_2-C_1)$	-58.077 °
$\tau(H_{12}-O_{11}-C_3-C_2)$	53.5886 °
$\tau(H_{13}-C_4-C_3-C_2)$	-159.939 °
$\tau(C_{14}-C_4-C_3-C_2)$	78.800 °
$\tau(O_{15}-C_4-C_3-C_2)$	-40.696 °
$\tau(H_{16}-O_{15}-C_4-C_3)$	156.281 °
$\tau(H_{17}-C_{14}-C_4-C_3)$	-39.029 °
$\tau(C_{18}-C_{14}-C_4-C_3)$	86.220 °
$\tau(O_{19}-C_{14}-C_4-C_3)$	-157.087 °
$\tau(H_{20}-O_{19}-C_{14}-C_4)$	205.371 °
$\tau(H_{21}-C_{18}-C_{14}-C_4)$	-74.073 °
$\tau(H_{22}-C_{18}-C_{14}-C_4)$	47.824 °
$\tau(H_{23}-C_{18}-C_{14}-C_4)$	-197.926 °
$\tau(H_{24}-O_{23}-C_{14}-C_4)$	226.437 °

Table 12. Calculated Wavenumbers $\bar{\nu}$ and Rotational Strengths R for D-Gulose [CHO-HCOH-HCOH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry.

$\bar{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
45.40	7.694
71.56	-17.700
88.10	-26.970
124.05	8.746
147.74	-15.408
191.37	11.904
239.46	24.759
273.96	18.995
296.95	-68.101
313.98	28.759
343.83	-53.984
377.39	-33.442
398.98	72.664
440.98	24.169
460.29	35.067
501.16	35.939
556.94	-21.939
602.27	-28.542
608.27	-56.998
647.02	87.904
662.58	47.570
688.08	13.323
763.22	-16.206
808.91	-169.490
888.99	-28.875
964.33	89.869
1028.24	-116.250
1076.71	-13.010
1105.81	-93.131
1121247	32.165
1154.24	-140.390
1157.42	59.488
1173.05	83.969
1181.00	57.143
1204.53	16.805
1209.36	-30.096
1282.93	-36.674
1375.98	9.311
1388.78	13.287
1400.73	16.256

Table 12. Calculated Wavenumbers $\dot{v}$ and Rotational Strengths R for D-Gulose [CHO-HCOH-HCOH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry. (Continued)

$\dot{v}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
1420.70	20.677
1433.79	-38.220
1457.28	0.217
1476.95	-6.379
1480.13	12.878
1489.31	-3.824
1515.00	80.734
1525.85	-73.688
1552.07	-47.641
1570.33	81.772
1587.72	12.502
1598.75	39.664
1677.01	5.633
1891.61	-4.013
3187.75	-1.361
3223.99	-20.478
3236.799	14.245
3245.72	4.197
3249.28	2.249
3277.18	6.404
3366.80	-2.064
3727.68	-54.202
3807.63	175.420
3811.27	-146.960
3853.34	-9.064
3882.86	2.045

Table 13. Optimized Geometry for D-Talose [CHO-HOCH-HOCH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level of Calculation. [The total energy = -679.532930595 a.u. and the dipole moment = 1.8084 D.]

geometrical coordinate	value of geometrical coordinate
r(C$_1$-C$_2$)	1.5078 A
r(C$_2$-C$_3$)	1.5348 A
r(C$_3$-C$_4$)	1.5239 A
r(C$_1$-H$_5$)	1.0831 A
r(C$_1$-O$_6$)	1.2125 A
r(C$_2$-O$_7$)	1.4375 A
r(C$_2$-H$_8$)	1.0852 A
r(O$_7$-H$_9$)	0.9733 A
r(C$_3$-H$_{10}$)	1.0771 A
r(C$_3$-O$_{11}$)	1.4398 A
r(O$_{11}$-H$_{12}$)	0.9686 A
r(C$_4$-H$_{13}$)	1.0816 A
r(C$_4$-C$_{14}$)	1.5166 A
r(C$_4$-O$_{15}$)	1.4588 A
r(O$_{15}$-H$_{16}$)	0.9715 A
r(C$_{14}$-H$_{17}$)	1.0803 A
r(C$_{14}$-C$_{18}$)	1.5221 A
r(C$_{14}$-O$_{19}$)	1.4459 A
r(O$_{19}$-H$_{20}$)	0.9694 A
r(C$_{18}$-H$_{21}$)	1.0775 A
r(C$_{18}$-H$_{22}$)	1.0789 A
r(C$_{18}$-H$_{23}$)	1.4527 A
r(O$_{23}$-H$_{24}$)	0.9659 A
ϕ(C$_3$-C$_2$-C$_1$)	112.267 °
ϕ(C$_4$-C$_3$-C$_2$)	113.967 °
ϕ(H$_5$-C$_1$-C$_2$)	112.932 °
ϕ(O$_6$-C$_1$-C$_2$)	124.830 °
ϕ(O$_7$-C$_2$-C$_3$)	115.587 °
ϕ(H$_8$-C$_2$-C$_3$)	106.021 °
ϕ(H$_9$-O$_7$-C$_2$)	109.246 °
ϕ(H$_{10}$-C$_3$-C$_2$)	108.073 °
ϕ(O$_{11}$-C$_3$-C$_2$)	110.318 °
ϕ(H$_{12}$-O$_{11}$-C$_3$)	108.218 °
ϕ(H$_{13}$-C$_4$-C$_3$)	108.852 °
ϕ(C$_{14}$-C$_4$-C$_3$)	117.876 °
ϕ(O$_{15}$-C$_4$-C$_3$)	104.567 °

Table 13. Optimized Geometry for D-Talose [CHO-HOCH-HOCH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level of Calculation. [The total energy = -679.532930595 a.u. and the dipole moment = 1.8084 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}\text{-}O_{15}\text{-}C_4)$	107.344 °
$\phi(H_{17}\text{-}C_{14}\text{-}C_4)$	109.942 °
$\phi(C_{18}\text{-}C_{14}\text{-}C_4)$	114.218 °
$\phi(O_{19}\text{-}C_{14}\text{-}C_4)$	103.237 °
$\phi(H_{20}\text{-}O_{19}\text{-}C_{14})$	107.834 °
$\phi(H_{21}\text{-}C_{18}\text{-}C_{14})$	111.631 °
$\phi(H_{22}\text{-}C_{18}\text{-}C_{14})$	109.872 °
$\phi(H_{23}\text{-}C_{18}\text{-}C_{14})$	106.826 °
$\phi(H_{24}\text{-}O_{23}\text{-}C_{14})$	108.288 °
$\tau(C_4\text{-}C_3\text{-}C_2\text{-}C_1)$	270.115 °
$\tau(H_5\text{-}C_1\text{-}C_2\text{-}C_3)$	163.569 °
$\tau(O_6\text{-}C_1\text{-}C_2\text{-}C_3)$	-15.531 °
$\tau(O_7\text{-}C_2\text{-}C_3\text{-}C_4)$	29.025 °
$\tau(H_8\text{-}C_2\text{-}C_3\text{-}C_4)$	151.980 °
$\tau(H_9\text{-}O_7\text{-}C_2\text{-}C_1)$	-219.104 °
$\tau(H_{10}\text{-}C_3\text{-}C_2\text{-}C_1)$	33.456 °
$\tau(O_{11}\text{-}C_3\text{-}C_2\text{-}C_1)$	149.562 °
$\tau(H_{12}\text{-}O_{11}\text{-}C_3\text{-}C_2)$	82.798 °
$\tau(H_{13}\text{-}C_4\text{-}C_3\text{-}C_2)$	-182.522 °
$\tau(C_{14}\text{-}C_4\text{-}C_3\text{-}C_2)$	52.509 °
$\tau(O_{15}\text{-}C_4\text{-}C_3\text{-}C_2)$	-66.776 °
$\tau(H_{16}\text{-}O_{15}\text{-}C_4\text{-}C_3)$	171.471 °
$\tau(H_{17}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-50.335 °
$\tau(C_{18}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	75.843 °
$\tau(O_{19}\text{-}C_{14}\text{-}C_4\text{-}C_3)$	-167.417 °
$\tau(H_{20}\text{-}O_{19}\text{-}C_{14}\text{-}C_4)$	202.120 °
$\tau(H_{21}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-73.938 °
$\tau(H_{22}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	48.590 °
$\tau(H_{23}\text{-}C_{18}\text{-}C_{14}\text{-}C_4)$	-196.983 °
$\tau(H_{24}\text{-}O_{23}\text{-}C_{14}\text{-}C_4)$	229.360 °

Table 14. Calculated Wavenumbers $\tilde{\nu}$ and Rotational Strengths R for D-Talose [CHO-HOCH-HOCH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry.

$\tilde{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
70.33	-1.073
88.58	2.215
121.26	90.347
124.59	0.866
134.51	-17.632
186.02	8.041
208.04	-6.055
256.86	40.146
283.44	-60.443
289.91	-37.186
333.12	-7.346
361.98	6.377
382.59	-63.215
404.18	-28.715
471.72	14.485
490.75	-183.000
515.65	96.981
530.55	-62.903
604.50	181.580
618.97	-273.840
649.78	11.199
717.08	-44.253
754.55	315.670
818.70	-178.480
854.03	84.908
956.65	12.669
997.75	-19.862
1048.74	-76.576
1081.61	8.223
1116.15	52.426
1127.96	17.210
1141.73	262.290
1167.54	42.336
1182.89	-70.291
1194.92	-38.622
1235.28	5.827
1298.32	-27.711
1330.79	51.844
1387.14	-76.571
1390.72	35.622

Table 14. Calculated Wavenumbers $\dot{\nu}$ and Rotational Strengths R for D-Talose [CHO-HOCH-HOCH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry. (Continued)

$\dot{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
1427.13	-97.781
1448.77	10.822
1456.25	18.058
1493.40	-25.488
1499.45	25.846
1510.55	53.015
1525.77	0.362
1534.03	15.901
1538.08	43.759
1549.25	54.800
1575.33	-20.722
1600.90	-22.521
1676.64	0.441
1902.08	-23.241
3211.87	-18.005
3224.22	-11.148
3247.58	2.542
3262.01	-12.929
3274.36	12.593
3316.85	-4.090
3331.98	3.878
3744.63	-132.020
3840.81	24.058
3855.95	-5.934
3861.43	15.522
3883.38	2.698

Table 15. Optimized Geometry for D-Galactose [CHO-HCOH-HOCH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level of Calculation. [The total energy = -679.541445638 a.u. and the dipole moment = 2.3610 D.]

geometrical coordinate	value of geometrical coordinate
r(C$_1$-C$_2$)	1.5097 A
r(C$_2$-C$_3$)	1.5309 A
r(C$_3$-C$_4$)	1.5263 A
r(C$_1$-H$_5$)	1.0824 A
r(C$_1$-O$_6$)	1.2081 A
r(C$_2$-O$_7$)	1.4327 A
r(C$_2$-H$_8$)	1.0835 A
r(O$_7$-H$_9$)	0.9748 A
r(C$_3$-H$_{10}$)	1.0787 A
r(C$_3$-O$_{11}$)	1.4342 A
r(O$_{11}$-H$_{12}$)	0.9701 A
r(C$_4$-H$_{13}$)	1.0815 A
r(C$_4$-C$_{14}$)	1.5227 A
r(C$_4$-O$_{15}$)	1.4484 A
r(O$_{15}$-H$_{16}$)	0.9703 A
r(C$_{14}$-H$_{17}$)	1.0851 A
r(C$_{14}$-C$_{18}$)	1.5231 A
r(C$_{14}$-O$_{19}$)	1.4418 A
r(O$_{19}$-H$_{20}$)	0.9692 A
r(C$_{18}$-H$_{21}$)	1.0810 A
r(C$_{18}$-H$_{22}$)	1.0782 A
r(C$_{18}$-H$_{23}$)	1.4508 A
r(O$_{23}$-H$_{24}$)	0.9661 A
ϕ(C$_3$-C$_2$-C$_1$)	110.249 °
ϕ(C$_4$-C$_3$-C$_2$)	111.551 °
ϕ(H$_5$-C$_1$-C$_2$)	113.767 °
ϕ(O$_6$-C$_1$-C$_2$)	122.750 °
ϕ(O$_7$-C$_2$-C$_3$)	108.909 °
ϕ(H$_8$-C$_2$-C$_3$)	110.862 °
ϕ(H$_9$-O$_7$-C$_2$)	106.603 °
ϕ(H$_{10}$-C$_3$-C$_2$)	109.297 °
ϕ(O$_{11}$-C$_3$-C$_2$)	107.693 °
ϕ(H$_{12}$-O$_{11}$-C$_3$)	107.145 °
ϕ(H$_{13}$-C$_4$-C$_3$)	107.335 °
ϕ(C$_{14}$-C$_4$-C$_3$)	113.403 °
ϕ(O$_{15}$-C$_4$-C$_3$)	108.296 °

Table 15. Optimized Geometry for D-Galactose [CHO-HCOH-HOCH-HOCH-HCOH-CH₂OH] Based on 3-21G Level of Calculation. [The total energy = -679.541445638 a.u. and the dipole moment = 2.3610 D.] (Continued)

geometrical coordinate	value of geometrical coordinate
$\phi(H_{16}-O_{15}-C_4)$	107.545 °
$\phi(H_{17}-C_{14}-C_4)$	110.631 °
$\phi(C_{18}-C_{14}-C_4)$	113.804 °
$\phi(O_{19}-C_{14}-C_4)$	104.776 °
$\phi(H_{20}-O_{19}-C_{14})$	108.330 °
$\phi(H_{21}-C_{18}-C_{14})$	112.346 °
$\phi(H_{22}-C_{18}-C_{14})$	109.692 °
$\phi(H_{23}-C_{18}-C_{14})$	107.311 °
$\phi(H_{24}-O_{23}-C_{14})$	106.388 °
$\tau(C_4-C_3-C_2-C_1)$	191.037 °
$\tau(H_5-C_1-C_2-C_3)$	228.642 °
$\tau(O_6-C_1-C_2-C_3)$	49.275 °
$\tau(O_7-C_2-C_3-C_4)$	75.229 °
$\tau(H_8-C_2-C_3-C_4)$	311.593 °
$\tau(H_9-O_7-C_2-C_1)$	-182.376 °
$\tau(H_{10}-C_3-C_2-C_1)$	-46.125 °
$\tau(O_{11}-C_3-C_2-C_1)$	70.004 °
$\tau(H_{12}-O_{11}-C_3-C_2)$	33.831 °
$\tau(H_{13}-C_4-C_3-C_2)$	-153.658 °
$\tau(C_{14}-C_4-C_3-C_2)$	84.278 °
$\tau(O_{15}-C_4-C_3-C_2)$	-34.593 °
$\tau(H_{16}-O_{15}-C_4-C_3)$	162.413 °
$\tau(H_{17}-C_{14}-C_4-C_3)$	-45.361 °
$\tau(C_{18}-C_{14}-C_4-C_3)$	79.217 °
$\tau(O_{19}-C_{14}-C_4-C_3)$	-163.561 °
$\tau(H_{20}-O_{19}-C_{14}-C_4)$	202.433 °
$\tau(H_{21}-C_{18}-C_{14}-C_4)$	-71.312 °
$\tau(H_{22}-C_{18}-C_{14}-C_4)$	50.668 °
$\tau(H_{23}-C_{18}-C_{14}-C_4)$	-194.821 °
$\tau(H_{24}-O_{23}-C_{14}-C_4)$	230.363 °

Table 16. Calculated Wavenumbers $\bar{\nu}$ and Rotational Strengths R for D-Galactose [CHO-HCOH-HOCH-HOCH-HCOH-CH₂OH] Based on 3-21G Level Optimized Geometry.

$\bar{\nu}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
51.33	8.801
71.63	-17.514
84.17	-7.235
115.93	13.698
132.32	30.486
169.48	9.564
211.48	-0.296
229.60	34.662
291.22	-29.660
297.39	-6.688
304.93	-7.343
353.18	-22.261
387.88	64.946
418.30	18.973
467.56	-2.292
493.99	16.492
553.13	-34.542
599.00	-134.040
602.77	-25.489
621.91	140.920
645.72	44.969
694.88	23.454
780.10	-84.671
854.36	52.170
877.61	-155.210
950.11	23.676
1029.35	-51.702
1055.71	108.330
1080.32	1.221
1108.96	-56.087
1120.68	121.870
1127.49	-25.820
1166.00	75.253
1193.84	4.681
1209.05	-114.680
1211.13	9.405
1281.81	-66.800
1339.53	-61.649
1363.47	-18.142
1388.16	-13.294

Table 16. Calculated Wavenumbers $\hat{v}$ and Rotational Strengths R for D-Galactose [CHO-HCOH-HOCH-HOCH-HCOH-CH$_2$OH] Based on 3-21G Level Optimized Geometry. (Continued)

$\hat{v}$ (cm^{-1})	R (x 10^{-44} esu^{2}cm^2)
1401.06	154.330
1443.56	-11.283
1467.21	-14.591
1484.97	22.162
1487.22	-3.895
1499.91	-33.622
1510.56	21.468
1522.77	-109.070
1532.76	46.972
1547.26	139.140
1575.45	-23.310
1585.29	-36.347
1668.27	3.130
1917.56	3.342
3196.82	3.669
3229.11	8.732
3231.65	-2.853
3245.34	-11.290
3256.15	24.825
3295.13	-15.329
3311.71	2.992
3760.62	19.701
3836.87	-63.016
3843.53	35.758
3859.40	-50.503
3879.73	2.144